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# MONTE CARLO SIMULATION OF BOSON SYSTEMS AT FINITE TEMPERATURE

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Finite temperature Monte Carlo simulation results for free bosons in the canonical ensemble are presented. A solution of the specific problems arising from the necessity to sum over all possible permutations of the particles is given.

The canonical partition function  $Z = \text{Tr } e^{-\beta H}$  of  $N$  bosons in a cube of volume  $V \equiv L^d$  can be obtained by calculating the approximant  $Z_m$  defined by

$$Z_m = c(\beta/m)^{-mdN/2} \sum_P \sum_{\{n_{i,j}\}} \int \prod_{i=1}^N \prod_{j=1}^m dx_{i,j} \exp[-S(\{x_{i,j}\}, \{n_{i,j}\})], \quad (1a)$$

where

$$S(\{x_{i,j}\}, \{n_{i,j}\}) = \frac{mM}{2\beta\hbar^2} \sum_{i=1}^N \sum_{j=1}^m (x_{i,j} - x_{i,j+1} + n_{i,j}L)^2 + \frac{\beta}{m} \sum_{j=1}^m \sum_{1 \leq i < i' \leq N} V(|x_{i,j} - x_{i',j}|), \quad (1b)$$

since one can prove that under very general conditions on the kinetic energy and potential energy operators  $Z = \lim_{m \rightarrow \infty} Z_m$  [1]. In (1) the sum over  $P$  runs over all possible permutations of the  $N$  particles,  $x_{i,m+1} \equiv x_{Pi,1}$  expresses the fact that we are taking the trace of a symmetrized density matrix, the sum over the  $n$ 's runs over all integers and takes into account that we are dealing with periodic boundary conditions,  $M$  is the mass of the particles,  $d$  is the spatial dimension and all unimportant constants have been absorbed in  $c$ . The index  $m$  accounts for the error made in neglecting a class of commutators of the kinetic and potential energy operators. In the limit  $m \rightarrow \infty$ ,  $Z_m$  becomes Feynman's path-integral representation of the boson canonical partition function [2,3].

As  $Z_m$  converges to  $Z$  if  $m$  increases and the same can be shown for all expectation values of interest, (1) can be used to calculate  $Z$  with increasing accuracy, provided the sums and  $mdN$ -dimensional integrals can be carried out. In principle, ratios of such integrals (i.e. expectation values of physical observables) can be computed by means of the Metropolis Monte Carlo method [4,5] since all mathematical conditions (see ref. [5]) are satisfied. However, due to the quantum nature of the model, several fundamental problems have to be solved before such a calculation can be carried out with any success.

A first difficulty is presented by the sum over all permutations. Unlike integrating over the  $x$ 's where it is easy to visualize the process of moving through phase space, summing over all permutations is more subtle. In particular it is not clear how to "walk" through this abstract space such that there is some guarantee that a representative part of it is sampled correctly. The algorithm not only has to work if the identity permutation is dominant (high

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temperature) or when all permutations are important (critical temperature) but for all intermediate cases as well. A second problem is related to the index  $m$  and the first term appearing in (1b). As we will have to let  $m$  increase, this term will force  $x_{i,j} \approx x_{i,j+1}$  and as noted before [6–8] this may prevent sizeable changes of the variables  $x_{i,j}$  and renders the computational scheme inefficient, even in the case where there is no sum over permutations. As in (1),  $x_{i,m+1} \equiv x_{p_i,1}$  this becomes even more problematic as it would be extremely difficult to change a permutation [7,9]. This by itself is remarkable since the index  $m$  is merely a vehicle for taking into account the error made by discretizing the path integral and changes in  $m$  should not have such a dramatic effect when we want to sum over all permutations. A third problem will arise because of the shape of the potential. It is well known that the harder the core of the potential, the larger  $m$  has to be to obtain sufficient accuracy [6–9]. A more ingenious way to deal with this particular problem is to use more sophisticated approximations than the one given by (1) [6,7].

In the present paper we concentrate on the first two problems. To solve the second one we propose to make a center-of-mass transformation with respect to the  $j$ -label. This can be done by repeated application of the identity

$$a(x-y)^2 + b(y-z)^2 = ab(x-z)^2/(a+b) + u^2, \quad u = y\sqrt{a+b} - (ax+bz)/\sqrt{a+b},$$

and changing the integration variables. The result is

$$Z_m = c' \beta^{-dN/2} \sum_P \sum_{\{n_i\}} \int_V \prod_{i=1}^N du_{i,1} \int_{-\infty}^{\infty} \prod_{i=1}^N \prod_{j=2}^m du_{i,j} \exp[-S(\{u_{i,j}\}, \{n_i\})], \quad (2a)$$

where

$$S(\{u_{i,j}\}, \{n_i\}) = \frac{M}{2\beta\hbar^2} \sum_{i=1}^N (u_{i,1} - u_{p_i,1} + n_i L)^2 + \sum_{i=1}^N \sum_{j=2}^m u_{i,j}^2 + \frac{\beta}{m} \sum_{j=1}^m \sum_{1 \leq i < i' \leq N} V(|x_{i,j} - x_{i',j}|), \quad (2b)$$

and

$$x_{i,j} = \left( \frac{2\beta\hbar^2}{mM} \right)^{1/2} \sum_{k=2}^j \frac{m-j+1}{m-k+1} \left( \frac{m-k+1}{m-k+2} \right)^{1/2} u_{i,k} + \frac{m-j+1}{m} (u_{i,1} + n_i L) + \frac{j-1}{m} u_{p_i,1}. \quad (2c)$$

The temperature dependent prefactor of the first term in (2c) only serves to reduce the statistical errors on the kinetic energy estimator and is not an essential part of the transformation itself as is seen by substituting  $u_{i,j} \rightarrow (mM/2\beta\hbar^2)^{1/2} u_{i,j}$  for all  $j \geq 2$ . Without this substitution (2c) leads to the same reduction of the variance on the kinetic energy as the one obtained by partial integration [10]. From (2b) it is clear that we have minimized the problem of accepting a move in permutation space as is illustrated by considering the free-boson case. In (1) the probability for accepting a change in permutation space depends strongly on  $\beta/m$  whereas in (2) it only depends on  $\beta$ . The price paid is that in the presence of interaction, one has to perform linear transformation (2c), which makes the algorithm non-local. As the number of operations for this transformation is proportional to  $mN$ , the labour involved is not too exhaustive.

We now turn to the first problem, moving through the space of all permutations. As with most Monte Carlo work, it is worthwhile to reduce analytically the number of integrals (or sums) as much as possible. To this end we rather sum over all possible cycles than over all permutations since this reduces the number of different integrals over the coordinates to a minimum [3,11]. This changes (2a) into

$$Z_m = c'' \beta^{-dN/2} \sum_{\{C_\lambda\}} \sum_{\{n_i\}} M(\{C_\lambda\}) \int_V \prod_{i=1}^N du_{i,1} \int_{-\infty}^{\infty} \prod_{i=1}^N \prod_{j=2}^m du_{i,j} \exp[-S(\{u_{i,j}\}, \{n_i\})], \quad (3a)$$

where the sum over  $C_\lambda$  is to be taken such that

$$\sum_{\lambda=1}^N \lambda C_{\lambda} = N, \quad (3b)$$

and the coefficient  $M(\{C_{\lambda}\})$  is given by [3,12]

$$M(\{C_{\lambda}\}) = N! \prod_{\lambda=1}^N \lambda^{-C_{\lambda}/C_{\lambda}!}. \quad (3c)$$

We emphasize that in going from (1) to (3) no approximation has been made.

Moving through the space consisting of integer numbers  $0 \leq C_{\lambda} \leq N$  subject to the constraint (3b) is the same as generating all possible partitionings of  $N$  [12]. Although there are many possibilities to do this not all of them will be useful in Monte Carlo work and therefore additional information of the relative importance of each configuration of cycles  $\{C_{\lambda}\}$  is welcome. For the free gas (3) has been used to calculate exactly all thermodynamic functions of the *canonical* ensemble [11] for small  $N$  and the information obtained in this way has been instrumental in developing a correct and efficient Monte Carlo algorithm for performing the sum over cycles ( $C_{\lambda}$ ) and coordinates ( $u_{i,j}$ ,  $n_{i,j}$ ).

In fig. 1 we compare the energy and specific heat obtained from Monte Carlo simulations of (3) for  $N = 32$ ,  $d = 3$  and  $\rho \equiv N/L^d = 0.0218$  (liquid  $^4\text{He}$  density) with the *exact* results for the *canonical* ensemble and conclude that there is excellent agreement. We have checked that this is not accidental by varying both  $N$  and  $\rho$ . At low temperatures it is essential to perform the sum over the  $n$ 's in order to reproduce the exact results. In fig. 2 we compare the same data with the standard *grand-canonical* results [13]. The energy is in excellent agreement with the rigorous result and the simulation also reproduces the main features of the specific heat. For the energy finite size effects are small but as can be expected this is not so for the specific heat if the temperature approaches the

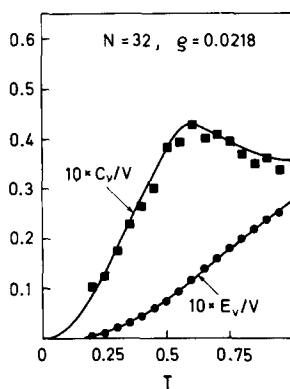


Fig. 1. Comparison of Monte Carlo simulation data for the energy (circles) and specific heat (squares) with exact result obtained from the canonical ensemble for a gas of non-interacting bosons. The temperature is measured in units such that  $\hbar^2/2k_B M = 1$ .

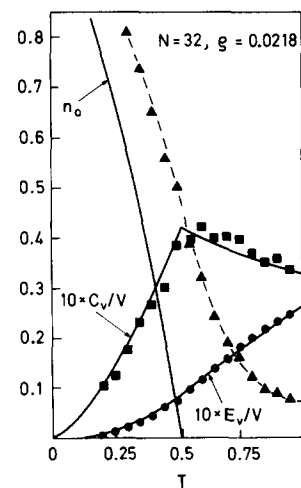


Fig. 2. Comparison of Monte Carlo simulation data for the energy (circles) and specific heat (squares) with exact results obtained from the grand-canonical ensemble for a gas of non-interacting bosons. The temperature is measured in units such that  $\hbar^2/2k_B M = 1$ . Also shown are the exact result for the condensate fraction of the infinite system ( $\rho_0$ ) and Monte Carlo data (triangles) for the corresponding quantity of the canonical ensemble. The dashed line is a guide to the eye only.

critical point. Also shown are Monte Carlo data for the condensate fraction  $n_0 \equiv n_{q=0}$  which in the limit  $V \rightarrow \infty$  will approach the condensate fraction of the infinite system from above. From fig. 2 it is clear that  $N = 32$  is too small for this upper bound to yield a good approximation for the condensate fraction of the infinite system. It is important to mention that except for the temperature and the seed of the random sequence, all other parameters of the simulation program have been kept fixed for all runs and no "fine-tuning" is necessary to obtain the agreement shown in fig. 1. Therefore we may conclude that the Monte Carlo algorithm for performing the sum over cycles is working correctly.

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### References

- [1] M. Reed and B. Simon, *Methods of modern mathematical physics*, Vols. 1, 2 (Academic Press, New York, 1972, 1975), and references therein.
- [2] R.P. Feynman and A.R. Hibbs, *Quantum mechanics and path integrals* (Mc-Graw-Hill, New York, 1965).
- [3] R.P. Feynman, *Statistical mechanics* (Benjamin, New York, 1972).
- [4] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, *J. Chem. Phys.* 21 (1953) 1087.
- [5] J.M. Hammersley and D.C. Handscomb, *Monte Carlo methods* (Methuen, London, 1964).
- [6] G. Jacucci, *NATO Workshop on Monte Carlo methods in quantum problems*, ed. M.H. Kalos (Reidel, Dordrecht, 1984), and references therein.
- [7] E.L. Pollock and D.M. Ceperley, *Phys. Rev.* B30 (1985) 2555.
- [8] M. Sprik, M.L. Klein and D. Chandler, *Phys. Rev.* B31 (1985) 4234.
- [9] M. Takahashi and M. Imada, *J. Phys. Soc. Japan* 53 (1983) 963.
- [10] M.F. Herman, E.J. Bruskin and B.J. Berne, *J. Chem. Phys.* 76 (1982) 5150.
- [11] H. de Raedt and A. Lagendijk, *Phys. Rep.*, to be published.
- [12] M. Abramowitz and I.A. Stegun, *Handbook of mathematical functions* (Dover, New York, 1965).
- [13] K. Huang, *Statistical mechanics* (Wiley, New York, 1963).